Multi-channel Characterization and Electrically-driven Migration of the Subsurface Hydrogen on Rutile TiO_2(110)-1×1 by nc-AFM/STM/KPFM at 78 K

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Subsurface defects are drawing increased research interest recently due to its dramatic modification on the physical and chemical properties of the nanoscale materials [1, 2]. Therefore, the understanding of the subsurface defects becomes important in clarifying the catalytic mechanism of titanium dioxide. In this study, for the first time, we have systematically investigated and deliberately manipulated the subsurface hydrogen H_{sub} on reduced rutile TiO_2(110)-1×1 with atomic resolution by a combination of noncontact atomic force microscopy (nc-AFM), scanning tunneling microscopy (STM) and Kelvin probe force microscopy (KPFM) at 78 K. Four different configurations of the H_{sub}, including the monomer, dimer, trimer and tetramer H_{sub}, are clearly characterized and distinguished. Specifically, it is experimentally demonstrated that the H_{sub} is negatively charged by the bright contrast of the H_{sub} in the KPFM image. In addition, we also demonstrate the ability to reversibly migrate the H_{sub} between the subsurface and surface layers, which is electrically driven by controlling the voltage pulse with different polarities. The underlying mechanism of the reversible cross-layer migration process can be explained by the electron excitation of the H_{sub} induced by the inelastic tunneling electrons and the local electric filed effect in the tunneling junction [3]. Our study provides a good reference for the systematic investigation and unprecedented manipulation approach of the subsurface defect at the single atom level and potentially have an overriding effect on revolutionizing the investigation and technological applications of the metal oxides.

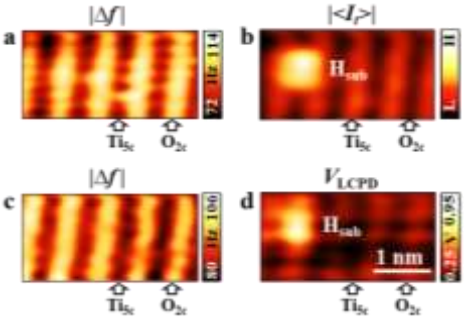

Figure 1. Characterization of the dimer of subsurface hydrogen H_{sub} on reduced rutile TiO_2(110)–1 × 1 surface by nc-AFM/STM/KPFM measurement at the same area in constant-height mode.

References

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